Evaluating Attenuated Total Reflectance Infrared and Near Infrared Spectroscopy for Classifiying *M. musculus* Grave Soil in the Presence of Clothing Material

Authors

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Introduction

- Clothing encountered in forensic casework can provide evidence assisting in victim identification and establishing the time elapsed for unattended death scenes.
- The presence, type and, weight of clothing can delay or enhance progression through the decomposition stages.[1]
- Recent works highlight the potential to identify and track degradation patterns of carrion-associated clothing, accumulation and composition of cadaveric fluids that are absorbed assisting in post-mortem interval (PMI) estimation.[2-3]
- Cadaveric fluid induces a succession of the soil's physical and chemical properties known as the cadaver decomposition island (CDI).[4]
- The subsequent impact of clothing on the temporal and lateral development of CDI should be reflected in physicochemical in the surrounding soil in a burial scenario.
- Attenuated total reflectance Fourier transform infrared (ATR-FTIR) and near-infrared (NIR) spectroscopy lend themselves to forensic applications in that they require only a small aliquot of sample material and little preparation while being non-destructive, rapid, portable, and reproducible.

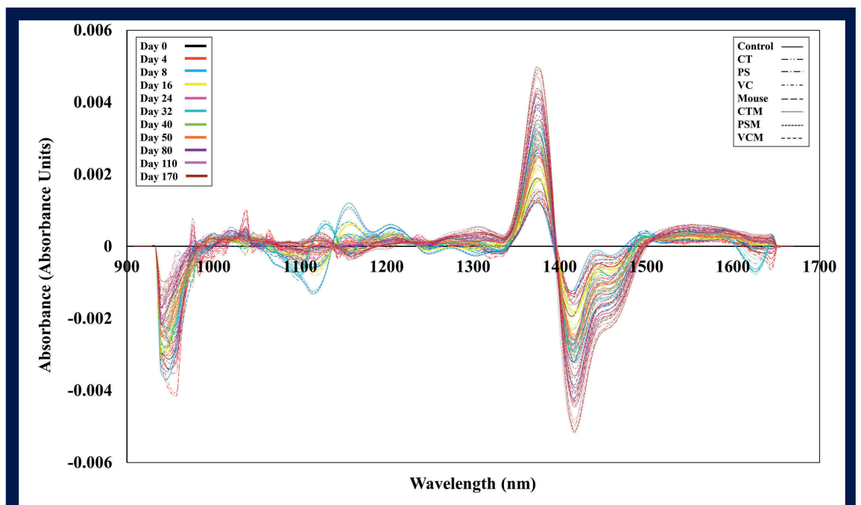

Figure 1. MSC-D2 treated NIR spectra from all soil samples.

Findings

- FTIR spectra and PC1 loadings plot highlight the variation seen as a result of bands at ~3010 cm^{-1}, 2920 cm^{-1}, and ~2850 cm^{-1} of the lipid methylene chain, (Figure 5a).[2-3]
- Delineation between 1100 and 1500 cm (Figure 5b) was associated with C-O stretching of volatile organic compounds (VOCs) that produce the characteristic smell of death such as ethers (1220-1260 cm^{-1}), esters (1100-1300 cm^{-1}) and carboxylic acids (1250-1450 cm^{-1}). [2-3]
- PCA scores plot of all FTIR spectra highlight differentiation of grave soil containing murine remains was more accurate within the inital 32 days post-burial, (Figure 4).
- NIR loadings plot highlights that 83.67% of the variation between samples was due to water II, the first overtone of the OH stretching (~1420 nm) and water III in the 1155 nm region, (Figure 7).[5]
- PCA scores plot of all NIR spectra demonstrates temporal differentiation between soils containing *M. musculus* and fabric controls (Figure 6).

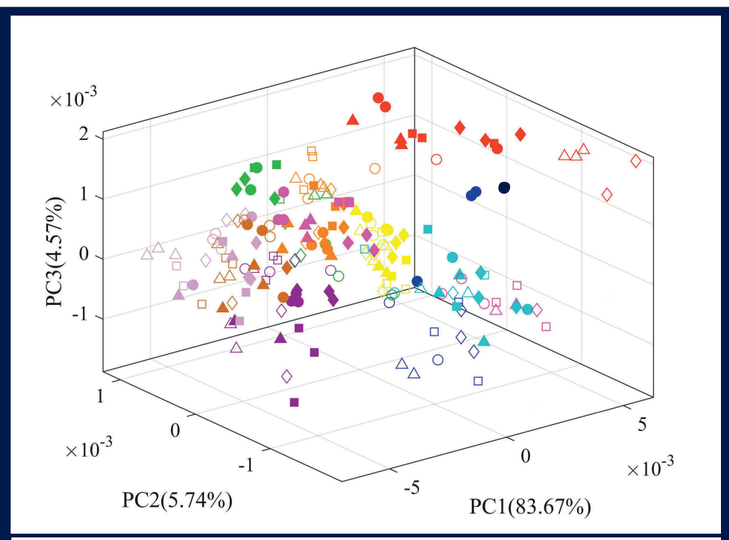

Figure 6. PCA scores plot of all MSC-D2 NIR spectra from grave soil containing: cotton (open circle), polyester (open square), viscose (open diamond) and control soils (open circle). Samples containing *M. musculus* carrion are represented by filled markers: unwrapped (circle), cotton-wrapped (triangle), polyester-wrapped (square) and viscose-wrapped (diamond) sampled on days **0**, **4**, **8**, **16**, **24**, **32**, **40**, **50**, **80**, **110** and **170**.

Objective

The aim of this study was to utilise non-destructive attenuated total reflectance Fourier transform infrared (ATR-FTIR) and near infrared (NIR) spectroscopic techniques to locate, identify and differentiate *Mus musculus* gravesoil in the presence of different clothing.

Methodology

- 24 burial microcosms were created including un clothed *M. musculus* and those wrapped in cotton, polyester and viscose.
- Soil samples were collected on days 0,4,8,16,24,32,40,50, 80,110 and 170.
- FTIR spectra was taken from 1-2 mg of soil within a range of 4000 – 400 cm^{-1} using Spectrum BX FT-IR spectrometer (Perkin Elmer, MA, USA) with a spectral resolution of 4 cm^{-1} averaged over 64 scans.
- NIR spectra were obtained on the JDSU microNIR 1700 pro-spectrometer (VIAVI Solutions, Arizona, USA) within a range of 900 – 1700 nm.
- All spectra were baseline corrected with Multiplicative Scatter Correction (MSC) and smoothed Savitzky-Golay 2nd derivative prior to analysis.
- Spectral visualisation, interpretation and principal component analysis was applied using Matlab 2019a.

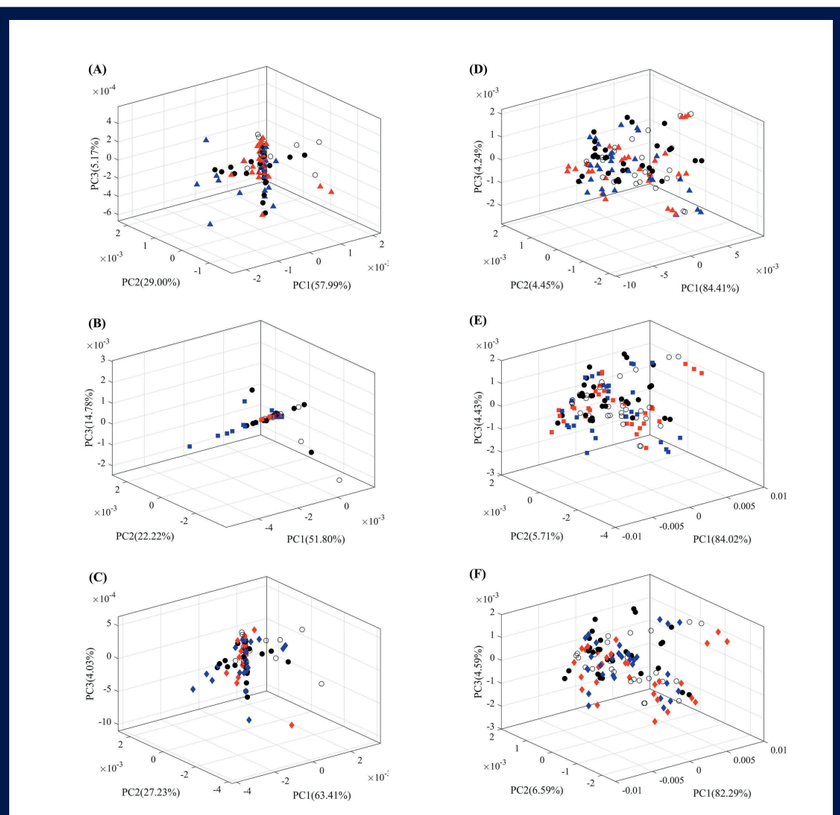

Figure 3. (A-C) PC scores plot of MSC-D2 treated FTIR spectra comparisons of 3100 cm-1 - 2700 cm-1 range from grave soil with unwrapped *M. musculus* (black circle); cotton only (red triangle); cotton wrapped *M. musculus* (blue triangle) (polyester only (red square); polyester wrapped *M. musculus* (blue square) viscose only (red diamond); viscose wrapped *M. musculus* (diamond). **(D-F)** PC scores plot of cotton MSC-D2 treated NIR spectra comparisons from grave soil with unwrapped *M. musculus* (black circle); cotton only (red triangle); cotton wrapped *M. musculus* (blue triangle), polyester only (red square); polyester wrapped *M. musculus* (blue square) viscose only (red diamond); viscose wrapped *M. musculus* (diamond). Open black circles indicate soil-only controls.

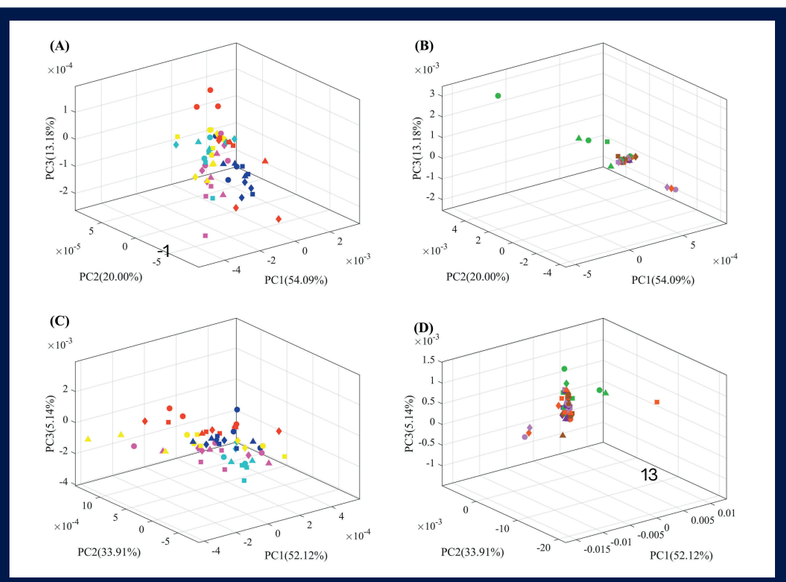

Figure 4. PCA scores plot of all MSC-D2 FTIR spectra containing a *M. musculus* carrion including: unwrapped (circle), cotton-wrapped (triangle), polyester-wrapped (square) and viscose-wrapped (diamond) *M. musculus* **(A)** expanded 3100 cm-1 - 2700 cm-1 region sampled on days **0**, **4**, **8**, **16**, **24**, **32** **(B)** expanded 3100 cm-1 - 2700 cm-1 region sampled on days **40**, **50**, **80**, **110** and **170** **(C)** expanded 1500 cm-1 - 1000 cm-1 region sampled on days **0**, **4**, **8**, **16**, **24**, **32** **(D)** expanded 1500 cm-1 - 1000 cm-1 region sampled on days **40**, **50**, **80**, **110** and **170**.

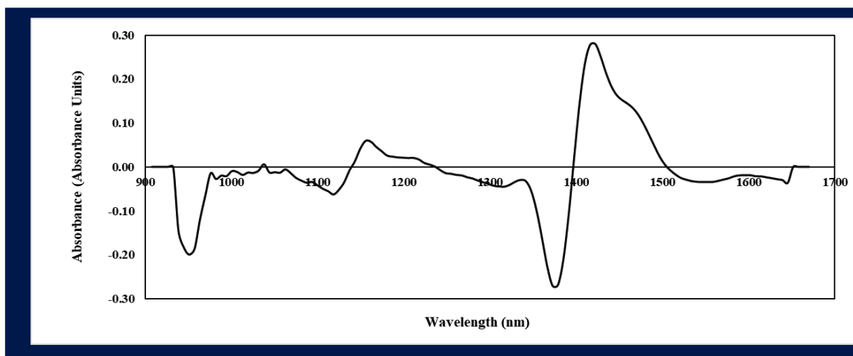

Figure 7. PC loadings plot of all MSC-D2 NIR spectra demonstrating the first principal component.

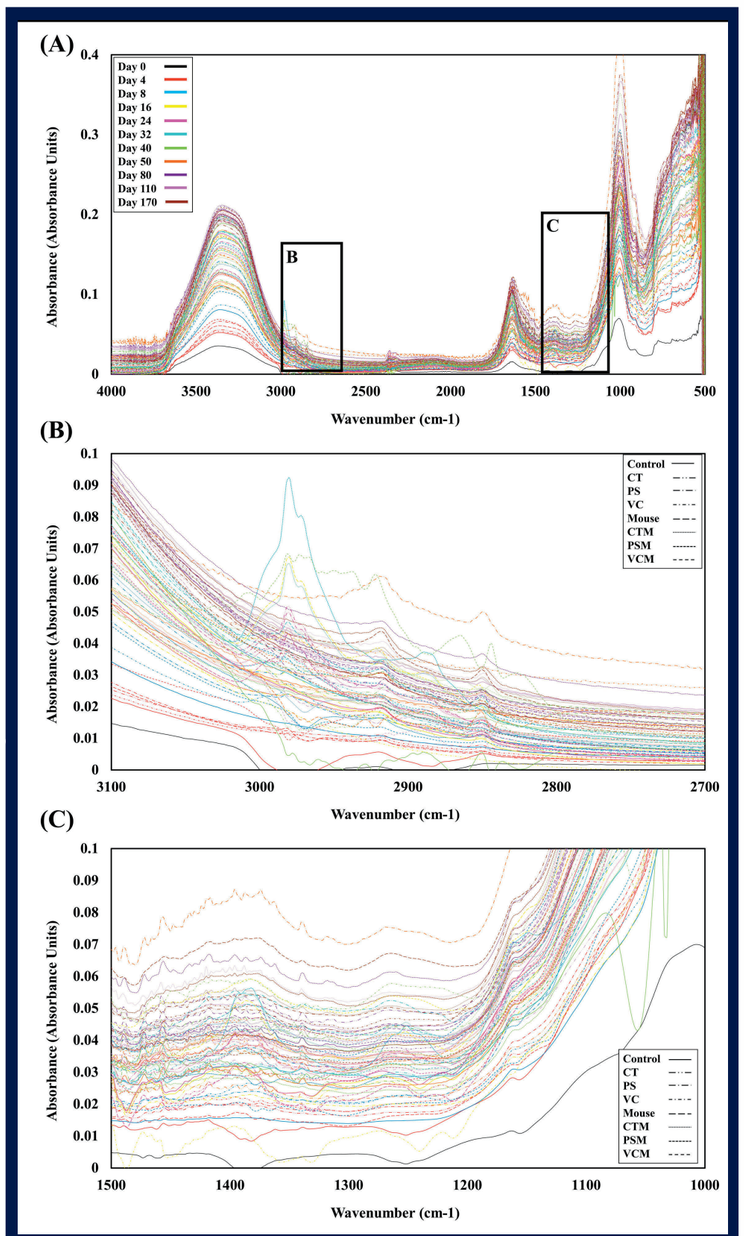

Figure 2. FTIR spectra of soil samples over **(A)** full range **(B)** 3100 cm-1 - 2700 cm-1 **(C)** 1500 cm-1 - 1000 cm-1 regions.

Conclusions

- Detection of simulation burial soils with FTIR was more accurate in the initial 32 days of deposition, with characteristic lipid and VOC compounds being able to be tracked.
- The portability and non-destructive nature of NIR is ideal for forensic casework application, in this study its ability to provide temporal information over 170-days of a burial in differing clothing has been demonstrated.
- The lack of identification of previously described lipid and amide bands at ~1760 cm^{-1} and 1680 cm^{-1}, respectively suggests that the size of the study model may have impacted the creating of a detectable CDI into the soil microcosm.

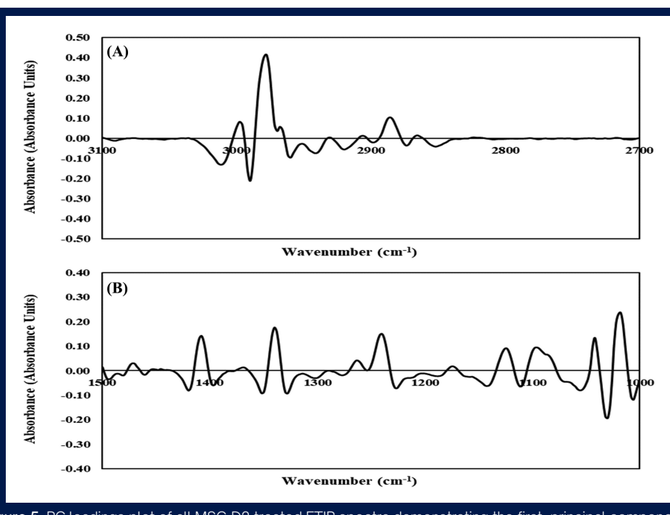

Figure 5. PC loadings plot of all MSC-D2 treated FTIR spectra demonstrating the first principal components for **A)** 3100 cm-1 - 2700 cm-1 **(B)** 1500 cm-1 - 1000 cm-1 regions.

References

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